

The surface energy and stress of metals

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We investigated surface properties of metals by performing first-principles calculations. A systematic database was established for the surface relaxation, surface energy (γ), and surface stress (τ) for metallic elements in the periodic table. The surfaces were modeled by multi-layered slab structures along the direction of low-index surfaces. The surface energy γ of simple metals decreases as the atomic number increases in a given group, while the surface stress τ has its minimum in the middle. The transition metal series show parabolic trends for both γ and τ with a dip in the middle. The dip occurs at half-band filling due to a long-range Friedel oscillation of the surface charge density, which induces a strong stability to the Peierls-like transition. In addition, due to magnetic effects, the dips in the $3d$ metal series are shallower and deeper for γ and τ , respectively, than those of the $4d$ and $5d$ metals. The surface stress of the transition metals is typically positive, only Cr and Mn have a negative τ for the (100) surface facet, indicating that they are under compression. The light actinides have an increasing γ trend according to the atomic number. The present work provides a useful and consistent database for the theoretical modelling of surface phenomena.

Keywords: Surface relaxation; Surface energy; Surface stress; Density-functional theory calculations; Metals

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1. Introduction

The surface energy (γ) and the surface stress (τ) are regarded as fundamental quantities to understand surface-related phenomena. In liquids, the surface energy and the surface stress are equal to each other. On the other hand, they differ in solids and we have $\tau_{ij} - \gamma\delta_{ij} = \partial\gamma/\partial\varepsilon_{ij}$ with the strain ε_{ij} on the surface plane. For high symmetry surfaces, the scalar surface stress τ can be introduced for the average stress. These surface parameters strongly depend on the crystalline structure [1] and the geometry of solid surfaces have continuously been an important subject of surface science.

Metals can transform surface structures and/or modify structural parameters from those of ideally as-truncated crystals due to the layer relaxation and reconstruction. For the layer relaxation, experimental results have shown that the top layer of transition metal surfaces tends to relax inward [2], while outward relaxation can arise for some noble metals. The top layer relaxation usually induces sub-surface layer relaxations. Several theoretical models have been proposed to explain the relaxation behaviors. Punkkinen *et al.* [2] elucidated the development of models for transition metals. Here, we extend previous results [3, 4] by a systematic approach to the layer relaxation and γ and τ of metal surfaces. It is shown that the layer relaxation is connected to γ and τ by a quadratic relationship and a linear relationship, respectively [1, 2].

Presently, the direct measurement of the surface quantities γ and τ is not easy. Accordingly, most of the available data have been obtained from the extrapolation of measurements on liquid phases, which is limited to isotropic crystals and not feasible for a specific surface orientation [5, 6]. Therefore, theoretical surveys of these properties have been crucial in the subject. Among several theoretical methods, two techniques are routinely used. Semi-empirical molecular dynamics methods, which are fast and computationally economical, have been helpful to understand trends of surface energetics for various materials [7-12], while leaving some doubts of reliability and accuracy. In contrast, first-principles methods are computationally expensive but provide reliable data. Thus, they have been widely spreading for a broad scope of materials research with the rapid development of computing resources. Intensive first-principles studies on the surface energies of metals have been reported by several workers [13-20], and there exist some results on various surface facets of metals determined with different methods [1-4, 21-25]. Here we should mention the database by Vitos *et al.* [4], which during the last two decades presented the most complete reference for surface energy and surface energy anisotropies of sixty metals from the periodic table. Vitos *et al.* [4] used the full-charge density linear muffin-tin orbitals (FCD-LMTO) method, which ensured sufficient accuracy for the surface excess energies but was not suitable to study the surface relaxation and surface stress. The purpose of

this paper is to revise and complement the previous works by compiling first-principles data for layer relaxation, surface energy, and surface stress for the low-index surfaces and thus providing an up-to-date and reliable database for metallic elements in the periodic table. We briefly describe the applied computational schemes in Section 2 and discuss results in Section 3.

2. Calculation methods

2.1. Surface energy and surface stress

The surface energy γ is defined by the reversible work per surface area to form a surface,

$$\gamma = \frac{E^s - E^b}{A}, \quad (1)$$

where E^s is the total energy of the system with surface, E^b is the total energy of the bulk system without surface, and A is the surface area. The number of atoms in the system is considered to be conserved. The surface stress τ is a tensorial quantity defined by the reversible work per surface area to stretch the surface in an elastic way and can be expressed in the form of the Shuttleworth equation [26],

$$\tau_{ij} = \frac{1}{A} \frac{\partial(A\gamma)}{\partial \varepsilon_{ij}} = \gamma \delta_{ij} + \frac{\partial \gamma}{\partial \varepsilon_{ij}}, \quad (2)$$

where τ_{ij} is the surface stress tensor, ε_{ij} is the in-plane surface strain tensor, and δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for otherwise). All the quantities in Eqs. (1) and (2) are evaluated for unstrained lattice, viz., $\varepsilon_{ij} = 0$.

The two surface parameters γ and τ depend on the layer relaxation in general. In order to understand the main relaxation effects, here we assume top layer relaxation only which actually gives the most significant effects compared to the subsurface layers. Accordingly, we have the inter-layer distance λ at the surface, which is different from the bulk value λ_0 . With the in-plane biaxial strain ε [27, 28] and the ratio of the change of the inter-layer distance at the surface to the layer distance in the bulk $\delta = (\lambda - \lambda_0)/\lambda_0$, the slab energy of a multi-layered system relative to the bulk energy is formally given by

$$E^s(\varepsilon, \delta) - E^b(\varepsilon) \cong E^s(0, 0) - E^b(0) + A_0 \left(\tau_0 \varepsilon + \frac{1}{2} \gamma_\varepsilon \varepsilon^2 + \frac{1}{2} \gamma_\delta \delta^2 + \tau'_0 \varepsilon \delta \right), \quad (3)$$

where τ_0 , γ_ε , γ_δ , and τ'_0 are the expansion coefficients, and A_0 is the surface area of the undistorted lattice. The slab energy $E^s(0, 0)$ corresponds to the layer-relaxed structure in equilibrium. Note that the bulk energy $E^b(\varepsilon)$ does not depend upon δ and only the second and higher order terms in ε appear. Therefore, the term linear in δ vanishes on the right side of the expansion.

Taking into account an infinitesimal strain $\varepsilon \rightarrow 0$, we can identify the surface energy and surface stress from the terms of Eq. (3) as

$$\begin{aligned} & \gamma(\delta) \\ \cong & \gamma(0) \\ & + \frac{1}{2} \gamma_\delta \delta^2 \end{aligned} \quad (4)$$

and

$$\begin{aligned} & \tau(\delta) \\ \cong & \tau(0) \\ & + \tau'_0 \delta, \end{aligned} \quad (5)$$

where $\gamma(0) = \{E^s(0, 0) - E^b(0)\}/A_0$ and $\tau(0) = \tau_0$ by definition, and τ'_0 is the derivative of $\tau(\delta)$ at $\delta = 0$. Thus it is found that the surface stress is more strongly (linearly) dependent on the layer relaxation than the surface energy (quadratically) [1, 2].

In order to evaluate the surface stress, a slab formed by a number of parallel atomic layers is usually considered and embedded in vacuum. The bulk structure is relaxed to the equilibrium to obtain the lattice parameters. With the equilibrium inter-layer distance λ_0 , multi-layer relaxation calculations are performed along the perpendicular direction to the surface plane. From the relaxed slab geometry, we elongate the lattice vectors within the surface plane by ε while keeping the inter-layer distances fixed. This deformation can be represented by the strain tensor,

$$\begin{aligned} & \varepsilon_{ij} \\ = & \begin{bmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & 0 \end{bmatrix}. \end{aligned} \quad (6)$$

We usually carry out calculations of E^s and E^b with a few small deformations, for example, $\varepsilon = 0$,

± 0.01 , and ± 0.02 and fit them to a quadratic polynomial

$$E^{s/b}(\varepsilon) \cong E^{s/b}(0) + c_1^{s/b} \varepsilon + c_2^{s/b} \varepsilon^2 , \quad (7)$$

where $c_1^{s/b}$ and $c_2^{s/b}$ are the coefficients of fitting. Then, the surface stress is determined from the linear coefficients of the slab and bulk energies as

$$\tau = \frac{c_1^s - c_1^b}{4A} . \quad (8)$$

The factor 4 comes from the double-sided surfaces of the slab and the homogeneous in-plane deformation [22, 27]. Finally we mention that the difference between the surface stress and the surface energy ($\tau - \gamma$) has previously been proposed as a measure of the driving force for surface reconstruction (see Refs. [2, 21] and references therein).

2.2. Numerical details

All calculations were performed within density-functional theory (DFT) [29]. To describe the electronic system with DFT, one needs to solve the one-electron Kohn-Sham problem [30] accurately and efficiently. In the present work, we employed the project augmented wave (PAW) method [31] as implemented within the Vienna Ab initio Simulation Package (VASP) [32, 33]. The exchange-correlation interaction was described by the generalized gradient approximation (GGA) [34, 35]. All calculation results including layer relaxation and surface stress were considered in comparison with previous theoretical and experimental data. Especially, the surface energy results of the PAW method were compared mainly with those obtained by the full-charge-density (FCD) approach within the linear muffin-tin orbitals (LMTO) method [36-39].

For $3d$ and $4d$ metals, the slab model of the surface consisted of 8 atomic layers for the face-centered cubic (fcc) (111) and (100) surfaces, 12 atomic layers for the body-centered cubic (bcc) (110) and the hexagonal close-packed (hcp) (0001) surfaces, and 16 atomic layers for the bcc (100) surfaces. For $5d$ metals, the slabs were 10 atomic layers thick except the bcc and fcc (100) facets, which were composed of 12 layers. A sufficiently thick vacuum region (approximately 10 \AA) separated the two surfaces. Spin polarization was considered for the $3d$ elements. Chromium was treated as an antiferromagnetic state with $B2$ structure [40] and Fe, Co, and Ni as ferromagnetically ordered. Manganese was calculated with its complex antiferromagnetic structure (α -Mn) with 58 atoms in the unit cell. The (110) surface

of α -Mn [41] was modeled by a slab containing 130 atoms separated by vacuum layers of thickness 12.2 Å. The Brillouin zone sampling was done with the Monkhorst–Pack scheme [42]. The plane wave cut-off energy was chosen as 450 ~ 500 eV for $3d$ metals, 340 ~ 460 eV for $4d$ metals, and 350 eV for $5d$ metals. All surfaces were subjected to surface layer relaxation, but surface reconstruction was not considered. Finally, for all surface facets the surface stress was determined through isotropic biaxial in-plane strains.

3. Results and discussion

The calculated results of the equilibrium bulk lattice constant, c/a ratio, surface relaxation, surface energy, and surface stress are listed in Tables 1–5 for simple metals, $3d$, $4d$, $5d$ metals, and light actinides, respectively. Below we discuss all sets of data separately.

3.1. Simple metals

For the alkali metals, we observe that the layer relaxation rapidly decays with the distance from the surface. The first layer relaxation is dominantly negative and the other layer relaxations are smaller by one order of magnitude. The top layer relaxation is significant, $d_{12} = -4.33\%$ for Li, small $d_{12} = -0.98\%$ for Na, and almost negligible for K, Rb, and Cs. This follows the trend of the atomic radius that increases from Li, Na, K, Rb to Cs.

The alkaline-earth metals and the other divalent sp metals including Zn and Cd show a layer relaxation in the opposite direction. The layer relaxation is positive for Be and Mg and becomes negative for Ca, Sr, and Ba in order of the atomic radius (see Table 1). The first layer relaxation also becomes smaller from 0.69% for Zn to 0.10% for Cd. These results are different from those of the alkali metals, where the relaxation pattern changes from negative values to positive ones as the atomic radius increases. It is also interesting to note that the relaxation trend of the most close-packed surface is rather independent on the bulk crystalline structure of metals. Moreover, as is evident from Table 1, the present PAW results for the layer relaxation are consistent with the previous theoretical and experimental data existing for Na, Be, Mg, Al, and Pb.

Figure 1 shows the surface energy of simple metals having sp valence electrons. The present results from the PAW method are mostly in good agreement with those of the FCD-LMTO method [4]. The surface energy of simple metals is found to be smaller than 1 J/m² except 1.77 J/m² for Be. As the atomic number increases, the surface energy decreases in each group of the periodic table. This might have a similar physical origin as the layer relaxation in Table 1. Especially for the alkali metals crystallizing in the bcc structure, it is clear that the larger the layer relaxation is, the larger the surface

energy is. For comparison, Fig. 1 contains the range of previously reported data from other theoretical and experimental approaches. The present surface energy values are mostly within the range of previous data. Though for Be, Mg, Al, and Pb the ranges are rather scattered, but in general they exhibit the trends of decreasing surface energy according to the increase of atomic numbers, as the present PAW results demonstrate.

Differently from the surface energy, the surface stress of simple metals is somewhat scattered; see Fig. 2. For the alkali metals, the surface stress is well bounded and between -0.29 J/m^2 and 0.12 J/m^2 , which are the values for K and Na, respectively. Beryllium has the largest surface stress $\tau = 2.99 \text{ J/m}^2$ among the considered simple metals. The surface stress of the alkaline-earth metals decreases from Be and Mg to Ca and increases again to Sr and Ba, forming the minimum value of $\tau = -0.85 \text{ J/m}^2$ for Ca. Although it is not as apparent as the case of the alkaline-earth metals, the surface stress of the alkaline metals also shows a shallow minimum for K. In addition, the difference between the surface stress and energy ($\tau - \gamma$) is positive for Be, Mg, Zn, Cd, Al, In and Tl, which exhibit an outward layer relaxation.

3.2. Transition metals

The lattice parameters, the surface energy, and the surface stress are listed in Tables 2–4 for $3d$, $4d$, and $5d$ transition metals, respectively. It is understood that the open surface structure, the (100) surface of bcc and fcc, induces more severe layer relaxation than the close-packed surfaces, the (110) and (111) surface of bcc and fcc, respectively. The layer relaxation is most pronounced for the first layer and usually declines within 2–3 surface layers, similarly to the simple metals. However, Friedel oscillations of the interlayer distance [43-45] screening the surface perturbation can persist to larger depth in some cases. For example, both Tc and Re are half-filled in the $4d$ and $5d$ series, respectively, and their layer relaxation slowly diminishes leading to only $d_{12}/d_{34} \sim 0.45$.

Aside from magnetic influences, the top layer relaxation of the three transition metal series as a function of the d -occupation is similar. Chromium is antiferromagnetically ordered in the ground state and iron has a ferromagnetic ground state. The calculated top layer relaxations for the bcc (110) facets of Cr and Fe are only -1.95% and -0.05% , respectively. These values are remarkably smaller in magnitude than those of adjacent non-magnetic $3d$ metals, for example, $d_{12} = -5.24\%$ for V. Molybdenum and tungsten share the same number of valence electrons with Cr and their top layer relaxations are $d_{12} = -4.74\%$ and -3.76% for Mo and W, respectively. Also, the (0001) surfaces of Ru and Os, which have the same valence electron number as Fe, relax as much as $d_{12} = -3.96\%$ and -3.79% , respectively. Hence, magnetic interactions and in particular the excess magnetic pressures near

the surface are likely to prevent significant layer relaxation of the surfaces. These trends are also consistently found in the other listed theoretical and experimental data. Most of the top layer relaxation data of the (110) surface of Fe and Cr are below 1% in magnitude, while those of Mo and W amount up to about 4%.

In addition, the behavior of Mn is quite noticeable. For the (110) facet, the α -Mn structure has a less dense layer between the first and the third surface layer, which are relatively close-packed. The inter-layer distance between the loosely-packed second layer and the third layer is small, which eventually gives a too large value of $d_{23} = 12.30\%$. Therefore, we reconsider this structure discarding the relaxation of d_{23} and obtain the first two inter-layer relaxations for α -Mn as $d_{13} = 0.99\%$ and $d_{34} = -1.83\%$, which are close in size to the results of Cr and Fe. Thus, the close-packed surfaces of the magnetic $3d$ metals exhibit unusually small layer relaxations and the positive magnetic pressure around the free surfaces would be the main cause of the phenomena of small relaxations.

One may also expect that the surface energy of a given element can be related to its cohesive energy as both of them scale with the bonding energy between constituent atoms. Especially, for transition metals, the surface energy per surface atom is roughly about 1/6 of the cohesive energy in bond-cutting models [17, 46]. Thus, the surface energy and the cohesive energy approximately follow the same trend in each of the three transition metal series.

In Fig. 3, we show the surface energies of $3d$, $4d$, and $5d$ transition metals. The surface energy of each period exhibits an approximately parabolic shape as a function of the d -electron occupation. When comparing the $4d$ with the $5d$ series, the surface energy of the $5d$ transition metals is larger than that of the $4d$ metals for the same valency, except at the end points. For the two elements bounding the $3d$ transition metal series, a higher surface energy is observed in comparison to that of the $4d$ and $5d$ metals. The data of both the PAW and the FCD-LMTO method are consistent in these main features and have an approximately parabolic shape. Most of the data point are found within the range of previously reported datasets. Specifically, many experimental surface energies lie in between the values of the PAW and FCD-LMTO methods or very close to them. We note that the FCD-LMTO results show higher surface energy values than the PAW partly due to the top-layer-only relaxation in the FCD-LMTO calculations.

The nearly parabolic shape of the surface energy across each transition metal series originates from the bonding nature of d -band electrons. Up to an approximately half-filled valance d -band, electrons predominantly occupy the bonding states enhancing the cohesive energy. After filling all the bonding

states, anti-bonding states start to be occupied, which lowers the cohesive energy. The Friedel model reflects this fact and explains the d -electron contribution to the cohesion of transition metals. According to the model, the surface energy of transition metals undergoes a parabolic variation with atomic number [47]. The surface energy estimated from the measured surface tension of liquid metals also verifies the parabolic trend of transition metals [6].

Looking into the details, each curve obtained from the PAW method shows a dip in the middle. It is more pronounced in the $4d$ and $5d$ metals than in the $3d$ metals. The elements in the middle of the transition metal series, Mn, Tc, and Re, have half-filled d -bands. As mentioned above, these elements exhibit charge-density oscillations at the surface. These will stabilize the close-packed surface of Tc and Re more easily leading to the lower surface energies compared to their neighboring elements. Furthermore, the correlation between the d -electrons is strong at the half-filled state and induces a stability to a Peierls-like bi-layer coupling. On the other hand, the effect is less pronounced in the bulk, resulting in a decreased value of the cohesive energy. We suggest that this mechanism introduces a dip in the parabolic surface energy curves.

Figure 4 shows the surface stress of transition metals. As one can see, most of the present PAW results are close to the preexisting data, and both of them show similar trends across each period. However, the ranges of the previous theoretical data for Pt and the experimental data for Pd and Cu are rather far from the present result. These disagreements may arise from the overestimation of surface stress by semi-empirical MEAM technique, and from the errors in lattice contraction measurement, for theoretical and experimental cases, respectively.

We also found that for the $4d$ and $5d$ metals, the surface stress as a function of the d -occupation varies similarly to the surface energy. For the early transition metals, the surface stress of the $5d$ metals is comparable to that of the $4d$ metals, whereas the other $5d$ metals have larger surface stresses than those of the $4d$ metals. The surface stress across the $4d$ and $5d$ transition metal series is approximately parabolic-shaped with a dip at approximately half d -band filling. Once again, the local minima are attributed to surface charge-density oscillations.

However, it is very interesting that the surface stress of the $3d$ transition metals behaves very differently from that of the $4d$ and $5d$ metals. As shown in Fig. 4, the surface stress of the $3d$ metals forms a deep sink instead of a shallow dip. Moreover, chromium and manganese have negative surface stress, $\tau = -0.32 \text{ J/m}^2$ and -0.22 J/m^2 , respectively, for the bcc (100) surface, which for Cr is thermodynamically more stable than the (110) surface (see Table 2). These findings mean that the bcc

(100) surfaces of Cr and Mn are under compression and tend to expand the in-plane lattice constant relative to the bulk one. The surface stresses of Fe, Co, and Ni are also lower than those of the isoelectronic elements of the $4d$ and $5d$ series. In order to understand this difference, we note that magnetic order occurs only in the $3d$ metals. The magnetic moment magnitude of Cr, Mn, Fe, Co, and Ni is enhanced at the surface due to the reduced coordination number. This enhanced surface magnetism impedes significant surface layer relaxation, which would otherwise be large in the absence of spin polarization. The lesser layer relaxation would not give rise to a big change in the surface energy, because the surface energy change is of second order in the layer relaxation as shown in Eq. (4). On the contrary, the surface stress depends linearly on the layer relaxation, Eq. (5). Therefore, the impeded layer relaxation due to the magnetism can greatly affect the surface stress as observed in the $3d$ transitional metals.

3.3 Light actinides

Examining the data in Table 5, for the multi-layer relaxation of some low-index surfaces of light actinides, we see that the relaxation decays rather fast with the distance from the surface. In addition, as the atomic number increases, the surface energy decreases. This was also reported in previous works [4, 48].

4. Conclusion

We have established a database of low-index surface properties for various metallic elements by employing a density-functional theory approach. Comparing with previous studies, the present work provides more complete and perhaps more accurate values of the surface energy and also embraces the multi-layer relaxation effects and the values of the surface stress. We expect that the database will be accessed as a useful reference in order to comprehend various kinds of surface phenomena of metallic materials.

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Table 1. Calculated surface relaxation (d_{ij}), surface energy (γ), and surface stress (τ) of simple metals. d_{ij} is given in percentage, γ and τ are in units of J/m². The calculated lattice constants a are listed with the structure information, in Å. Previously reported data are also tabulated, with their annotation numbers starting as T and E , for theoretical and experimental cases, respectively.

Metal	Structure a (c/a)	Surface	Relaxation			γ	τ	$\tau - \gamma$
			d_{12}	d_{23}	d_{34}			
Li	bcc 3.44	(110)	-4.33	-0.23	0.61	0.49 0.56 ^{T1} , 0.53 ^{T2} 0.50 ^{T3} , 0.54 ^{T4} , 0.46 ^{T5} , 0.46 ^{T6} 0.52 ^{E1} , 0.53 ^{E2} 0.47 ^{E3}	-0.13	-0.62
Na	bcc 4.19	(110)	-0.98 -1.6±0.5 ^{T7} -0.33±0.33 ^{E4}	0.38 0.0±0.5 ^{T7}	0.01 0.6±0.8 ^{T7}	0.21 0.25 ^{T1} , 0.22 ^{T2} 0.31 ^{T5} , 0.24 ^{T6} 0.25 ^{T7} , 0.26 ^{E1} 0.26 ^{E2} , 0.23 ^{E3}	0.12	-0.09
K	bcc 5.28	(110)	-0.01	0.01	0.00	0.11 0.14 ^{T1} , 0.11 ^{T2} 0.12 ^{T5} , 0.13 ^{T6} 0.15 ^{E1} , 0.13 ^{E2} 0.14 ^{E3}	-0.29	-0.40
Rb	bcc 5.67	(110)	0.00	0.00	0.00	0.08 0.10 ^{T1} , 0.10 ^{T2} 0.09 ^{T5} , 0.11 ^{T6} 0.09 ^{T8a} , 0.12 ^{T8b} 0.12 ^{E1} , 0.11 ^{E2} 0.11 ^{E3}	0.03	-0.05
Cs	bcc 6.15	(110)	0.00	0.00	0.00	0.06 0.08 ^{T1} , 0.06 ^{T2} 0.07 ^{T5} , 0.08 ^{T6} 0.10 ^{E1} , 0.10 ^{E2} 0.08 ^{E3}	0.04	-0.02
Be	hcp 2.26 (1.58)	(0001)	2.78 3.17 ^{T9a} 2.74 ^{T9b} 3.9 ^{T10} 3.2 ^{T11} 2.6 ^{T12} 5.8 ^{E5} 3.1±0.7 ^{E6}	0.84 1.15 ^{T9a} 1.18 ^{T9b} 2.2 ^{T10} 1.0 ^{T11} 0.8 ^{T12} -0.2 ^{E5} 1.4±0.7 ^{E6}	0.47 0.65 ^{T9a} 0.77 ^{T9b} 0.4 ^{T11} 0.2 ^{E5} 0.9±0.9 ^{E6}	1.77 1.83 ^{T1} , 2.12 ^{T5} 1.67 ^{T9a} , 2.01 ^{T9b} 1.92 ^{T10} , 2.1 ^{T13} 1.53 ^{T14} , 1.63 ^{E1} 2.70 ^{E2}	2.99	1.22
Mg	hcp 3.19 (1.62)	(0001)	1.45 2.04 ^{T9a} 1.13 ^{T9b} 1.24 ^{T15a} 1.18 ^{T15b} 1.5±0.1 ^{T16} 1.8 ^{T17}	0.26 1.13 ^{T9a} 0.31 ^{T9b} 0.21 ^{T15a} 0.36 ^{T15b} 0.5±0.1 ^{T16} 0.2 ^{T17}	-0.35 0.72 ^{T9a} 0.21 ^{T9b} -0.72 ^{T15a} -0.73 ^{T15b} 0.1±0.1 ^{T16} -0.3 ^{T17}	0.55 0.79 ^{T1} , 0.64 ^{T5} , 0.30 ^{T9a} , 0.35 ^{T9b} 0.56 ^{T15a} , 0.62 ^{T15b} 0.64 ^{T17} , 0.89 ^{T18} 0.29 ^{T14} , 0.79 ^{E1} 0.76 ^{E2} , 0.82 ^{E3}	0.88	0.33

Ca	fcc 5.52	(111)	1.9 ± 0.3^{E7}	0.8 ± 0.4^{E7}	-0.4 ± 0.5^{E7}	0.41 0.57 ^{T1} , 0.51 ^{T2} 0.35 ^{T5} , 0.50 ^{T19} 0.50 ^{E1} , 0.49 ^{E2} 0.48 ^{E3}	-0.85	-1.25
			-1.82	0.57	0.24			
Sr	fcc 6.02	(111)	-1.84	0.70	0.10	0.35 0.43 ^{T1} , 0.40 ^{T2} 0.44 ^{T8a} , 0.55 ^{T8b} 0.29 ^{T5} , 0.37 ^{T19} 0.42 ^{E1} , 0.41 ^{E2} 0.38 ^{E3}	-0.48	-0.83
Ba	bcc 5.03	(110)	-2.04	0.92	0.08	0.31 0.38 ^{T1} , 0.37 ^{T2} 0.26 ^{T5} , 0.38 ^{E1} 0.37 ^{E2} , 0.35 ^{E3}	0.03	-0.28
Zn	hcp 2.66 (1.57)	(0001)	0.69	-0.65	-0.10	0.32 0.99 ^{T1} , 0.20 ^{T14} 0.99 ^{E1} , 0.99 ^{E2} 0.91 ^{E3}	1.44	1.12
			1.0 ± 1.0^{E8}					
Cd	hcp 3.05 (1.87)	(0001)	0.10	-0.11	0.01	0.21 0.59 ^{T1} , 0.14 ^{T14} 0.76 ^{E1} , 0.74 ^{E2} 0.73 ^{E3}	1.07	0.86
Al	fcc 4.04	(111)	0.96	-0.56	0.12	0.82 1.20 ^{T1} , 0.93 ^{T2} 1.27 ^{T5} , 0.75 ^{T15a} 0.91 ^{T15b} , 1.10 ^{T19} 0.67 ^{T20} , 0.94 ^{T21} 1.12 ^{T22} , 0.62 ^{T24} 0.96 ^{T25} , 0.71 ^{T26} 0.96 ^{T27} , 0.91 ^{T28} 1.14 ^{E1} , 1.16 ^{E2} 1.28 ^{E3}	1.64	0.82
			1.35 ^{T15a}	0.54 ^{T15a}	1.06 ^{T15a}			
			1.35 ^{T15b}	0.54 ^{T15b}	1.04 ^{T15b}			
			1.04 ^{T20}	-0.54 ^{T20}	0.19 ^{T20}			
			1.18 ^{T21}	-0.40 ^{T21}	0.22 ^{T21}			
			1.0 ^{T22}	0.0 ^{T22}				
			1.00 ^{T23}	-0.07 ^{T23}				
			2.73 ^{T24}	0.25 ^{T24}	0.02 ^{T24}			
			1.7 ± 0.3^{E9}	0.5 ± 0.7^{E9}				
			2.2 ± 1.3^{E10}					
			0.9 ± 0.5^{E11}					
			1.3 ± 0.8^{E12}					
			1.4 ± 0.5^{E13}					
			In	bct 3.37 (1.44)	(100)			
(110)	0.27	-0.72			0.68	0.36 0.56 ^{T1} , 0.70 ^{E1} 0.68 ^{E2} , 0.60 ^{E3}	1.96	1.6
Tl	hcp 3.57 (1.57)	(0001)	0.83	-1.61	0.15	0.29 0.30 ^{T1} , 0.70 ^{T18} 0.60 ^{E1} , 0.58 ^{E2} 0.49 ^{E3}	0.57	0.28
Sn	diamond 6.65	(100)	2.04	0.54	0.12	0.88 0.61 ^{T1} , 0.71 ^{E1} 0.68 ^{E2} , 0.61 ^{E3}	0.43	-0.45
		(111)	-2.96	0.99	-0.82			

Pb	fcc	(111)	-4.71	1.93	0.51	0.27	0.72	0.45
	5.03		-3.75 ^{T24}	0.77 ^{T24}	-0.15 ^{T24}	0.32 ^{T1} , 0.60 ^{T19}	0.64 ^{T24}	
			-4.8 ^{T30}	1.8 ^{T30}	-0.3 ^{T30}	0.36 ^{T24} , 0.21 ^{T28}	0.82 ^{T32}	
			-6.9 ^{T31}	0.6 ^{T31}	-0.7 ^{T31}	0.28 ^{T30} , 0.56 ^{T31}		
			-3.5±1.0 ^{E14}	0.5±1.4 ^{E14}	1.6±1.8 ^{E14}	0.26 ^{T32} , 0.59 ^{E1}		
						0.60 ^{E2} , 0.52 ^{E3}		
						0.44±0.02 ^{E15}		

* calculated as bct structure, for (001) plane [4]

^{T1} FCD-LMTO, GGA [4]

^{T2} PAW, GGA (Perdew-Burke-Ernzerhof revised for solids (PBEsol)) [49]

^{T3} linear combination of Gaussian-type orbitals, GGA [50]

^{T4} pseudopotential, GGA [51]

^{T5} tight-binding (TB) LMTO, local density approximation (LDA) [3]

^{T6} semi-empirical, empirical electron surface model (EESM) [52]

^{T7} pseudopotential, LDA [53]

^{T8a} exact muffin-tin orbitals (EMTO), GGA (Perdew-Burke-Ernzerhof (PBE)) [54]

^{T8b} EMTO, LDA [54]

^{T9a} pseudopotential, GGA [55]

^{T9b} pseudopotential, LDA [55]

^{T10} linearized augmented plane-wave (LAPW), LDA [56]

^{T11} pseudopotential, LDA [57]

^{T12} pseudopotential, LDA [58]

^{T13} pseudopotential, LDA [59]

^{T14} semi-empirical, empirical electron theory (EEM) [60]

^{T15a} full-potential linearized augmented plane-wave (FP-LAPW), GGA [19]

^{T15b} FP-LAPW, LDA [19]

^{T16} pseudopotential, LDA [61]

^{T17} pseudopotential, LDA [62]

^{T18} semi-empirical, modified embedded-atom method (MEAM) [63]

^{T19} full-potential Korringa-Kohn-Rostoker (FKKR), LDA [64]

^{T20} pseudopotential, GGA [20]

^{T21} pseudopotential, LDA [65]

^{T22} pseudopotential, LDA [66]

^{T23} pseudopotential, LDA [67]

^{T24} semi-empirical, MEAM [11]

^{T25} pseudopotential, LDA [68]

^{T26} pseudopotential, LDA [69]

^{T27} pseudopotential, LDA [70]

^{T28} semi-empirical, EESM [71]

^{T29} linear combination of atomic orbitals (LCAO), LDA [72]

^{T30} pseudopotential, GGA [73]

^{T31} ultrasoft pseudopotential (USPP), GGA [74]

^{T32} pseudopotential, LDA [75]

^{E1} extrapolation from surface tension measurement [5]

^{E2} extrapolation from surface tension measurement [6]

^{E3} extrapolation from surface tension measurement [76]

^{E4} low-energy electron diffraction (LEED) [77]

^{E5} LEED [78]

^{E6} LEED [79]

^{E7} LEED [80]

^{E8} LEED [81]

^{E9} LEED [82]

^{E10} LEED [83]

^{E11} LEED [84]

^{E12} LEED [85]

^{E13} LEED [86]

^{E14} LEED [87]

^{E15} scanning tunneling microscopy (STM) [88]

Table 2. Calculated surface relaxation (d_{ij}), surface energy (γ), and surface stress (τ) of 3d transition metals. d_{ij} is given in percentage, γ and τ are in units of J/m². The calculated lattice constants a are listed with the structure information, in Å. Previously reported data are also tabulated, with their annotation numbers starting as T and E , for theoretical and experimental cases, respectively.

Metal	Structure a (c/a)	Surface	Relaxation			γ	τ	$\tau - \gamma$
			d_{12}	d_{23}	d_{34}			
Sc	hcp 3.32 (1.55)	(0001)	-2.58	1.19	0.29	1.26	0.73	-0.53
			-1.89±0.76 ^{E1}			1.83 ^{T1} , 0.82 ^{T2}		
Ti	hcp 2.94 (1.59)	(0001)	-0.04±0.19 ^{E2}			0.82 ^{T3} , 1.26 ^{T4}	0.65	-1.32
			-6.08±1.14 ^{E3}	-1.14±1.14 ^{E3}		1.28 ^{E4} , 1.16 ^{E5}		
			-7.7 ^{T5}	2.8 ^{T5}		2.63 ^{T1} , 1.95 ^{T2}		
			-6.84 ^{T6a}	2.82 ^{T6a}	-0.51 ^{T6a}	1.40 ^{T3} , 2.19 ^{T5}		
			-6.44 ^{T6b}	2.64 ^{T6b}	0.37 ^{T6b}	1.99 ^{T6a} , 2.27 ^{T6b}		
			-6.47 ^{T7}	4.01 ^{T7}	-0.68 ^{T7}	1.96 ^{T7} , 1.95 ^{T8}		
			-7.55 ^{T8}	2.86 ^{T8}	-0.94 ^{T8}	2.24 ^{T9} , 2.10 ^{E4}		
			-6.8 ^{T9}	1.2 ^{T9}		1.98 ^{E5} , 1.99 ^{E8}		
			-4.9 ^{E6}	1.4 ^{E6}	-1.1 ^{E6}			
			-2.14±2.14 ^{E7}					
V	bcc 2.99	(100)	-12.41	0.24	2.87	2.40	2.12	-0.28
			-9.0 ^{T10}	0.6 ^{T10}		3.03 ^{T1} , 3.4 ^{T10}		
		-6.67 ^{E9}	0.99 ^{E9}		2.68 ^{T11} , 3.00 ^{T12}			
					2.11 ^{T13} , 2.83 ^{T14}			
		(110)	-5.24	0.58	0.01	2.41	2.12	-0.29
			-0.93±0.93 ^{E10}			3.26 ^{T1} , 2.02 ^{T2}		
						2.66 ^{T11} , 1.62 ^{T13}		
						2.65 ^{T14}		
Cr	bcc* 2.87	(100)	-5.06	3.62	-1.04	3.06	-0.32	-3.38
			-0.17±0.55 ^{E11}			3.98 ^{T1} , 4.05 ^{T11}		
					3.37 ^{T13} , 2.42 ^{T14}			
					2.23 ^{T15} , 2.30 ^{E4}			
		(110)	-1.95	0.44	0.20	3.10	0.79	-2.31
			0.89±0.25 ^{E11}			2.89 ^{E5} , 2.35 ^{E8}		
						3.51 ^{T1} , 3.59 ^{T11}		
						2.60 ^{T13} , 2.23 ^{T14}		
Mn	bcc** 2.80 α -Mn 8.64	(100)				2.14	-2.24	-4.38
						1.57 ^{T15}		
		(110)	2.59			2.59	-0.22	-2.81
						3.10 ^{T1} , 2.80 ^{T15} , 2.80 ^{T15} , 2.80 ^{T15}		
						2.42 ^{T16} , 1.60 ^{E4}		
						1.59 ^{E5} , 1.54 ^{E8}		
Fe	bcc 2.84	(100)	-6.95	12.30	-1.83		1.39	-1.11
			($d_{13} = 0.99$)	($d_{34} = -1.83$)				
			-0.18	2.88	0.78	2.50	0.57^{T23a}	
			-1.89 ^{T17}	2.59 ^{T17}	0.21 ^{T17}	2.22 ^{T1} , 3.12 ^{T11}		

			-3.09 ^{T18}	2.83 ^{T18}	1.93 ^{T18}	2.66 ^{T13} , 2.57 ^{T14}	1.15 ^{T23b}	
			-3.03 ^{T19}	2.14 ^{T19}	3.11 ^{T19}	2.18 ^{T15} , 2.29 ^{T17}	0.23 ^{T24}	
			-3.6 ^{T20}	2.3 ^{T20}	0.4 ^{T20}	2.25 ^{T18} , 2.47 ^{T20}		
			0.35 ^{T21}	-0.14 ^{T21}		2.35 ^{T22} , 2.62 ^{T23a}		
			-0.21±2.09 ^{E12}	1.19±2.09 ^{E12}		3.07 ^{T23b} , 2.53 ^{T24}		
			-1.4±3 ^{E13}					
		(110)	-0.05	0.71	-0.15	2.45	1.56	-0.89
			-0.13 ^{T17}	0.20 ^{T17}	-0.06 ^{T17}	2.43 ^{T1} , 3.00 ^{T11}	1.91 ^{T24}	
			-0.11 ^{T18}	1.16 ^{T18}	1.14 ^{T18}	2.05 ^{T13} , 2.37 ^{T14}		
			-0.33 ^{T19}	0.89 ^{T19}	0.76 ^{T19}	2.66 ^{T15} , 2.27 ^{T17}		
			-0.1 ^{T20}	0.3 ^{T20}	-0.5 ^{T20}	2.25 ^{T18} , 2.37 ^{T20}		
			-0.35 ^{T25}	0.44 ^{T25}		2.25 ^{T22} , 2.46 ^{T24}		
			-0.36 ^{T26}	0.46 ^{T26}	-0.26 ^{T26}	2.29 ^{T25} , 2.43 ^{T26}		
			-0.08 ^{T27}	0.40 ^{T27}	-0.25 ^{T27}	2.43 ^{T28} , 2.41 ^{T29}		
			0.23 ^{T28}	0.77 ^{T28}	-0.20 ^{T28}	2.48 ^{E4} , 2.62 ^{E5}		
			-0.52 ^{T29}	0.43 ^{T29}	-0.29 ^{T29}	2.42 ^{E8}		
			1±2 ^{E14}	0.5±1 ^{E14}				
			0.5±2.0 ^{E15}					
Co	hcp 2.49 (1.62)	(0001)	-2.89	1.85	-0.72	2.11	2.20	0.09
			-2.55 ^{T30}	1.34 ^{T30}	-0.48 ^{T30}	2.78 ^{T1} , 2.86 ^{T3}		
			-2.93±0.98 ^{E16}	0.49±1.95 ^{E16}	-1.95±2.93 ^{E16}	2.99 ^{T4} , 2.74 ^{T15}		
			-2.1 ^{E17}	1.3 ^{E17}		2.55 ^{E4} , 2.52 ^{E5}		
						2.52 ^{E8}		
Ni	fcc 3.52	(100)	-3.74	0.55	0.04	2.22	1.73	-0.49
			-3.6 ^{T31}	1.4 ^{T31}	0.3 ^{T31}	2.43 ^{T1} , 2.61 ^{T11}	2.37 ^{T33}	
			-3.6 ^{T32}	1.0 ^{T32}		2.77 ^{T15} , 2.60 ^{T16}	2.39 ^{T37}	
			2.53 ^{T33}	0.08 ^{T33}	0.00 ^{T33}	2.19 ^{T31} , 2.48 ^{T32}		
			-3.7 ^{T34}	0.4 ^{T34}		2.42 ^{T33} , 2.25 ^{T36}		
			-2.7 ^{T35}					
			1.14±1.14 ^{E18}					
			-3.2±0.5 ^{E19}					
		(111)	-1.31	-0.09	0.11	1.92	2.16	0.24
			-1.02 ^{T30}	-0.25 ^{T30}	0.59 ^{T30}	2.01 ^{T1} , 2.28 ^{T8}	2.00 ^{T30}	
			-0.9 ^{T31}	0.0 ^{T31}	0.0 ^{T31}	2.69 ^{T15} , 2.27 ^{T16}	2.21 ^{T33}	
			-1.2 ^{T32}	0.1 ^{T32}		1.93 ^{T31} , 1.88 ^{T32}	2.23 ^{T37}	
			2.70 ^{T33}	0.05 ^{T33}	0.00 ^{T33}	2.02 ^{T33} , 1.95 ^{T36}		
			-2.1 ^{T34}	0.2 ^{T34}		2.03 ^{T38} , 2.45 ^{E4}		
			-1.5 ^{T35} , -0.6 ^{T38}			2.37 ^{E5} , 2.38 ^{E8}		
			-1.23±1.23 ^{E18}					
			0±1 ^{E20}					
Cu	fcc 3.64	(100)	-1.61	1.48	1.25	1.44	2.55	1.11
			-0.83 ^{T33}	0.04 ^{T33}	-0.00 ^{T33}	2.17 ^{T1} , 2.09 ^{T2}	2.10 ^{T33}	
			-3.6 ^{T34}	0.3 ^{T34}		1.81 ^{T11} , 1.92 ^{T16}	1.87 ^{T37}	
			-3.02 ^{T39}	0.08 ^{T39}	-0.24 ^{T39}	1.65 ^{T33} , 1.71 ^{T39}		
			-1.06 ^{T40}	-0.65 ^{T40}	1.28 ^{T40}	1.80 ^{T42} , 2.15 ^{T43}		
			-2.52 ^{T41}	0.84 ^{T41}	0.68 ^{T41}			
			-1.2 ^{E21}	0.9 ^{E21}				
			-2.4 ^{E22}	1.0 ^{E22}				
			-1.1±0.4 ^{E23}	1.7±0.6 ^{E23}				
			-2.1 ^{E24}	0.45 ^{E24}				

	-1.1 ^{E25}	1.7 ^{E25}				
	-1.0±0.4 ^{E26}	2.0±0.8 ^{E26}				
(111)	-0.31	0.04	0.31	1.30	1.87	0.57
	-1.19 ^{T6a}	-0.65 ^{T6a}	-0.24 ^{T6a}	1.95 ^{T1} , 1.96 ^{T2}	1.93 ^{T33}	
	-1.58 ^{T6b}	-0.73 ^{T6b}	-0.43 ^{T6b}	1.41 ^{T6a} , 1.92 ^{T6b}	1.73 ^{T37}	
	0.14 ^{T33}	-0.01 ^{T33}	0.00 ^{T33}	1.67 ^{T11} , 1.67 ^{T16}	0±0.45 ^{E30}	
	-2.0 ^{T34}	0.1 ^{T34}		1.41 ^{T33} , 1.59 ^{T39}		
	-1.27 ^{T39}	-0.64 ^{T39}	-0.26 ^{T39}	1.91 ^{T43} , 1.94 ^{T44}		
	0.56 ^{T40}	-0.07 ^{T40}	0.55 ^{T40}	1.83 ^{E4} , 1.70 ^{E5}		
	-0.60 ^{T41}	-0.18 ^{T41}	0.12 ^{T41}	1.79 ^{E8}		
	-0.7 ^{E27}	-0.6 ^{E27}	-0.8 ^{E27}			
	-0.3±1.0 ^{E28}					
	0.5 ~ 1 ^{E29}					

^{*} commensurable antiferromagnetic state with the B2 structure [40]

^{**} hypothetical ferromagnetic structure (unrelaxed)

^{***} calculated as fcc structure, for (111) plane

^{T1} FCD-LMTO, GGA [4]

^{T2} TB LMTO, LDA [3]

^{T3} semi-empirical, EEM [60]

^{T4} semi-empirical, MEAM [63]

^{T5} LAPW, LDA [89]

^{T6a} FP-LAPW, GGA [19]

^{T6b} FP-LAPW, LDA [19]

^{T7} ultrasoft pseudopotential (USPP), GGA [20]

^{T8} PAW, GGA (Perdew-Wang 91 (PW91)) [90]

^{T9} pseudopotential, LDA [91]

^{T10} FP-LAPW, LDA [92]

^{T11} PAW, GGA (PBEsol) [49]

^{T12} FP-LAPW, LDA [93]

^{T13} semi-empirical, EEM [94]

^{T14} semi-empirical, second nearest-neighbor MEAM [95]

^{T15} TB LMTO, LDA [96]

^{T16} semi-empirical, EESM [72]

^{T17} USPP, GGA (PW91) [97]

^{T18} USPP, GGA [98]

^{T19} USPP, GGA (in PW91) [99]

^{T20} PAW, GGA [100]

^{T21} pseudopotential, LDA [101]

^{T22} USPP, GGA (PW 91) [102]

^{T23a} EMTO, GGA (PBE) [103]

^{T23b} full-potential local-orbital (FPLO), PBE [103]

^{T24} EMTO, GGA (PBE) [104]

^{T25} USPP, GGA [105]

^{T26} PAW, GGA (PW91) [106]

^{T27} PAW, LDA [107]

^{T28} PAW, GGA(PBE) [108]

^{T29} PAW, GGA (PBE) [132]

^{T30} USPP, GGA (PW91) [109]

^{T31} USPP, GGA [110]

^{T32} PAW, GGA (PW91) [111]

^{T33} semi-empirical, MEAM [11]

^{T34} TB [112]

^{T35} TB [113]

^{T36} PAW, GGA (PBE) [114]

^{T37} USPP, GGA (PBE) [115]

^{T38} USPP, GGA (PW91) [116]

^{T39} pseudopotential, LDA [117]

^{T40} pseudopotential, LDA [118]

^{T41} FP-LAPW, GGA (PBE) [119]

^{T42} modified augmented plane-wave, LDA [120]

*T*₄₃ FKKR, LDA [64]
*T*₄₄ FP-LMTO, LDA [121]
*E*₁ LEED [122]
*E*₂ LEED [123]
*E*₃ LEED [124]
*E*₄ extrapolation from surface tension measurement [6]
*E*₅ extrapolation from surface tension measurement [76]
*E*₆ LEED [125]
*E*₇ LEED [126]
*E*₈ extrapolation from surface tension measurement [5]
*E*₉ LEED[127]
*E*₁₀ LEED [128]
*E*₁₁ LEED[129]
*E*₁₂ LEED [130]
*E*₁₃ LEED [131]
*E*₁₄ medium energy ion scattering (MEIS) [133]
*E*₁₅ LEED [134]
*E*₁₆ LEED [135]
*E*₁₇ LEED [136]
*E*₁₈ LEED [137]
*E*₁₉ Rutherford backscattering spectroscopy (RBS) [138]
*E*₂₀ MEIS [139]
*E*₂₁ LEED [140]
*E*₂₂ MEIS [117]
*E*₂₃ LEED [141]
*E*₂₄ LEED [142]
*E*₂₅ LEED [143]
*E*₂₆ LEED [144]
*E*₂₇ LEED [145]
*E*₂₈ LEED [146]
*E*₂₉ LEED [147]
*E*₃₀ lattice contraction experiment [148]

Table 3. Calculated surface relaxation (d_{ij}), surface energy (γ), and surface stress (τ) of 4d transition metals. d_{ij} is given in percentage, γ and τ are in units of J/m². The calculated lattice constants a are listed with the structure information, in Å. Previously reported data are also tabulated, with their annotation numbers starting as T and E , for theoretical and experimental cases, respectively.

Metal	Structure a (c/a)	Surface	Relaxation			γ	τ	$\tau - \gamma$
			d_{12}	d_{23}	d_{34}			
Y	hcp 3.65 (1.55)	(0001)	-2.37	0.94	0.21	1.00	1.00	0.00
			-3.66 ^{T1}			1.51 ^{T2} , 1.18 ^{T3a} 1.38 ^{T3b} , 0.68 ^{T4} 1.15 ^{T5,*} , 0.74 ^{T6} 1.13 ^{E1} , 1.03 ^{E2}	0.60 ^{T1}	
Zr	hcp 3.23 (1.61)	(0001)	-6.39	2.04	0.25	1.57	1.15	-0.42
			-2.77 ^{T1} -4.7 ^{T7} -6.3 ^{T8} , -1±2 ^{E3}	1.2 ^{T7}	1.0 ^{T7}	2.26 ^{T2} , 1.90 ^{T3a} 2.15 ^{T3b} , 1.53 ^{T4} 1.75 ^{T5,*} , 1.23 ^{T6} 2.04 ^{T7} , 1.73 ^{T8} 2.25 ^{T9} , 2.00 ^{E1} 1.73 ^{E2} , 1.91 ^{E4}	1.57 ^{T1}	
Nb	bcc 3.31	(110)	-4.21	0.60	-0.27	2.06	2.99	0.93
			-1.88 ^{T1} -3.7 ^{T5} -3.6 ^{T10}	-0.5 ^{T10}		2.69 ^{T2} , 2.32 ^{T3a} , 2.66 ^{T3b} , 1.64 ^{T4} 2.36 ^{T5} , 2.9 ^{T11} 2.32 ^{T12} , 2.39 ^{T13} 2.50 ^{T14} , 2.70 ^{E1} 2.49 ^{E2} , 2.67 ^{E4}	3.44 ^{T1}	
Mo	bcc 3.17	(100)	-12.44	-0.50	3.46	2.32	0.89	-1.43
			-4.69 ^{T1} -9.3 ^{T5} -6.3 ^{T10}	-0.7 ^{T10}		2.86 ^{T2} , 2.86 ^{T5} 3.1 ^{T11} , 2.63 ^{T12} 3.15 ^{T13} , 2.77 ^{T14}	1.79 ^{T1}	
Mo	bcc 3.17	(110)	-4.74	0.73	0.22	2.73	2.96	0.23
			-1.56 ^{T1} -3.9 ^{T5} -3.3 ^{T10} -4.3 ^{T15} -1.6±2.0 ^{E5}	-0.7 ^{T10} -0.2 ^{T15}	-0.4 ^{T15}	3.45 ^{T2} , 3.23 ^{T3a} 3.69 ^{T3b} , 3.18 ^{T4} 3.14 ^{T5} , 3.03 ^{T12} 2.54 ^{T13} , 2.92 ^{T14} 2.92 ^{T15} , 3.00 ^{E1} 2.07 ^{E2} , 2.91 ^{E4}	4.15 ^{T1}	
Mo	bcc 3.17	(100)	-13.05	4.20	-2.58	3.15	1.98	-1.17
			-4.36 ^{T1} -9.0 ^{T5} -6.9 ^{T10} -11.1 ^{T15} -9.5±3.0 ^{E6}	-1.1 ^{T10} 2.3 ^{T15} 1.0±2.0 ^{E6}	-1.7 ^{T15}	3.84 ^{T2} , 3.52 ^{T5} 3.49 ^{T12} , 3.32 ^{T13} 3.26 ^{T14} , 3.34 ^{T15}	3.27 ^{T1}	
Tc	hcp 2.76 (1.60)	(0001)	-6.70	5.23	-3.03	2.21	2.59	0.38
			-1.53 ^{T1}			3.69 ^{T2} , 3.25 ^{T3a} 3.86 ^{T3b} , 2.80 ^{T4} 2.63 ^{T5,*} , 2.66 ^{T6} 3.15 ^{E1}	3.48 ^{T1}	

Ru	hcp 2.73 (1.58)	(0001)	-3.96	0.12	0.10	2.52	3.15	0.63		
			-1.04 ^{T1}			3.93 ^{T2} , 3.47 ^{T3a}	4.75 ^{T1}			
			-3.80 ^{T16}	0.20 ^{T16}	0.44 ^{T16}	4.18 ^{T3b} , 3.32 ^{T4}	3.33 ^{T16}			
			-3 ^{T17}			2.99 ^{T5,*} , 3.0 ^{T17}				
			-4.0 ^{T18}			3.05 ^{E1} , 2.89 ^{E2}				
			-2.1 ^{E7}	-0.1 ^{E7}	0.5 ^{E7}	3.04 ^{E4}				
Rh	fcc 3.85	(100)	-4.05	0.42	0.34	2.35	2.35	0.00		
			-1.30 ^{T1} , -3.5 ^{T5}			2.80 ^{T2} , 2.90 ^{T4}	2.14 ^{T1}			
			-4.3 ^{T10}	0.6 ^{T10}		2.81 ^{T5} , 2.84 ^{T12}	4.30 ^{T19}			
			-4.5 ^{T19} , -5.1 ^{T20}			2.79 ^{T19} , 2.59 ^{T20}	3.15 ^{T21}			
			-3.4 ^{T21}			2.65 ^{T24} , 2.90 ^{T25}	2.04 ^{T27}			
			-3.8±0.2 ^{T22}	0.7±0.3 ^{T22}	0.6±0.3 ^{T22}	3.12 ^{T26}				
					0.2 ^{T23}	-0.04 ^{T23}	-0.04 ^{T23}			
					-6.9±1.0 ^{E8}	1.9±1.0 ^{E8}				
					1.0±0.9 ^{E9}					
					0.5±2.0 ^{E10}					
					-1.4±3.6 ^{E11}					
				(111)	-1.80	-0.74	0.63	2.01	2.73	0.72
			-0.20 ^{T1} , -2.5 ^{T5}			2.47 ^{T2} , 2.63 ^{T3a}	2.11 ^{T1}			
			-2.4 ^{T10}	0.3 ^{T10}		3.34 ^{T3b} , 2.78 ^{T4}	2.29 ^{T16}			
			-2.02 ^{T16}	-1.55 ^{T16}	-0.29 ^{T16}	2.53 ^{T5} , 2.44 ^{T12}	2.97 ^{T21}			
			-1.6 ^{T21}			2.59 ^{T25} , 2.65 ^{T26}				
			-1.7±0.2 ^{T22}	-0.3±0.1 ^{T22}	0.5±0.1 ^{T22}	2.70 ^{E1} , 2.61 ^{E2}				
			-1.6±0.8 ^{E9}			2.66 ^{E4}				
			-2±2 ^{E12}							
			-2.7±1.4 ^{E13}							
Pd	fcc 3.96	(100)	-1.33	-0.13	0.27	1.51	2.16	0.65		
			-0.75 ^{T1} , -0.6 ^{T5}			2.33 ^{T2} , 1.90 ^{T4}	1.69 ^{T1}			
			-4.2 ^{T10}	0.6 ^{T10}		1.86 ^{T5} , 1.84 ^{T12}	2.07 ^{T19}			
			-0.8 ^{T19} , -1.20 ^{T29}			1.79 ^{T19} , 2.22 ^{T26}	2.69 ^{T30}			
			-1.30 ^{T28}	-0.00 ^{T28}	0.35 ^{T28}	1.49 ^{T28} , 2.13 ^{T29}				
			-1.97 ^{T30}	0.17 ^{T30}	-0.01 ^{T30}	1.66 ^{T30} , 2.17 ^{T31}				
					0.29±1.54 ^{E14}	-0.77±1.54 ^{E14}	2.3 ^{E9}			
					0.3±2.6 ^{E15}					
				(111)	0.42	-0.32	-0.07	1.33	2.57	1.24
					0.28 ^{T1} , -0.1 ^{T5}			1.92 ^{T2} , 1.65 ^{T3a}	2.15 ^{T1}	
					-2.5 ^{T10}	0.3 ^{T10}		2.29 ^{T3b} , 1.88 ^{T4}	1.89 ^{T16}	
					0.55 ^{T16}	-0.06 ^{T16}	0.25 ^{T16}	1.64 ^{T5} , 1.59 ^{T12}	3.14 ^{T30}	
			0.25 ^{T28}	-0.34 ^{T28}	0.10 ^{T28}	2.01 ^{T26} , 1.31 ^{T28}	3.69 ^{T36}			
			-0.32 ^{T30}	-0.02 ^{T30}	-0.00 ^{T30}	1.38 ^{T30} , 1.89 ^{T31}	6.0±0.9 ^{E19}			
			-0.01 ^{T32a}	-0.41 ^{T32a}	-0.22 ^{T32a}	1.33 ^{T32a} , 1.87 ^{T32b}				
			-0.22 ^{T32b}	-0.53 ^{T32b}	-0.33 ^{T32b}	1.85 ^{T35} , 2.05 ^{E1}				
			-0.03 ^{T33}	0.08 ^{T33}	0.00 ^{T33}	1.99 ^{E2} , 2.00 ^{E4}				
			-0.10 ^{T34}							
			1.3±1.3 ^{E16}	-1.3±1.3 ^{E16}	2.2±1.3 ^{E16}					
			2.4±0.9 ^{E17}	0.7±0.9 ^{E17}	0.7±1.8 ^{E17}					
			0.0±4.4 ^{E18}							
Ag	fcc 4.16	(100)	-1.71	0.56	0.25	0.84	1.31	0.47		
			-1.08 ^{T1} , -1.9 ^{T5}			1.20 ^{T2} , 1.20 ^{T4}	0.88 ^{T1}			
			-4.5 ^{T10}	0.6		1.21 ^{T5} , 1.14 ^{T12}	1.68 ^{T19}			

	-1.04 ^{T30}	0.11 ^{T30}	-0.01 ^{T30}	1.12 ^{T19} , 1.40 ^{T26}	1.48 ^{T30}	
	-1.9 ^{T37}			1.09 ^{T30} , 1.03 ^{T31}		
	0±1.5 ^{E20}			1.24 ^{T37} , 1.27 ^{T38}		
				1.3 ^{E9}		
(111)	-0.30	-0.46	0.07	0.76	0.79	0.03
	0.16 ^{T1} , -1.4 ^{T5}			1.17 ^{T2} , 0.89 ^{T3a}	0.75 ^{T1}	
	-2.6 ^{T10}	0.1 ^{T10}		1.40 ^{T3b} , 1.12 ^{T4}	1.75 ^{T30}	
	0.94 ^{T30}	-0.07 ^{T30}	0.00 ^{T30}	1.21 ^{T5} , 1.07 ^{T12}	1.42±0.30 ^{E26}	
	-1.3 ^{T37}			1.25 ^{T26} , 1.09 ^{T30}		
	0.00±0.85 ^{E21}	0.00±1.27 ^{E21}		0.90 ^{T31} , 1.24 ^{T37}		
	-2.5 ^{E22} , -2~ ^{E23}			1.25 ^{E1} , 1.20 ^{E2}		
	0 ^{E24} , -2.5 ^{E25}			1.25 ^{E4}		

* calculated as fcc structure, for (111) layer

^{T1} exact muffin-tin orbitals, GGA [22]

^{T2} FCD-LMTO, GGA [4]

^{T3a} exact muffin-tin orbitals (EMTO), GGA (PBE) [65]

^{T3b} exact muffin-tin orbitals (EMTO), LDA [65]

^{T4} TB LMTO, LDA [3]

^{T5} FP-LMTO, LDA [17]

^{T6} semi-empirical, EEM [60]

^{T7} pseudopotential, LDA [149]

^{T8} LAPW, LDA [89]

^{T9} semi-empirical, MEAM [63]

^{T10} TB [112]

^{T11} FP-LAPW, LDA [150]

^{T12} PAW, GGA (PBEsol) [49]

^{T13} semi-empirical, EEM [94]

^{T14} semi-empirical, second nearest-neighbor MEAM [95]

^{T15} pseudopotential, LDA [151]

^{T16} USPP, GGA (PW91) [109]

^{T17} pseudopotentials, LDA [152]

^{T18} LAPW, LDA [153]

^{T19} FP-LMTO, LDA [154]

^{T20} LAPW, LDA [16]

^{T21} USPP, LDA [155]

^{T22} USPP, LDA [156]

^{T23} semi-empirical, MEAM [157]

^{T24} pseudopotentials, LDA [158]

^{T25} semi-empirical, MEAM [159]

^{T26} FKKR, LDA [64]

^{T27} USPP, GGA (PBE) [115]

^{T28} FP-LAPW, GGA [19]

^{T29} pseudopotentials, LDA [160]

^{T30} semi-empirical, MEAM [11]

^{T31} semi-empirical, EESM [71]

^{T32a} USPP, GGA [20]

^{T32b} USPP, LDA [20]

^{T33} FP-LAPW, GGA [161]

^{T34} FCD-LMTO, LDA and GGA [4, 48]

^{T35} USPP, LDA [162]

^{T36} LCAO [163]

^{T37} FP-LMTO, LDA [164]

^{T38} FP-LAPW, LDA [165]

^{E1} extrapolation from surface tension measurement [6]

^{E2} extrapolation from surface tension measurement [76]

^{E3} LEED [166]

^{E4} extrapolation from surface tension measurement [5]

^{E5} LEED [167]

^{E6} LEED [168]

^{E7} LEED [153]

E8 LEED [169]
E9 LEED [170]
E10 LEED [171]
E11 LEED [172]
E12 LEED [173]
E13 LEED [174]
E14 LEED [175]
E15 LEED [176]
E16 LEED [177]
E17 LEED [178]
E18 high energy ion scattering (HEIS) [179]
E19 measurement from metal clusters [180]
E20 LEED [181]
E21 LEED [182]
E22 MEIS [183]
E23 HEIS [184]
E24 LEED [185]
E25 MEIS [186]
E26 lattice contraction experiment [187]

Table 4. Calculated surface relaxation (d_{ij}), surface energy (γ), and surface stress (τ) of 5d transition metals. d_{ij} is given in percentage, γ and τ are in units of J/m². The calculated lattice constants a are listed with the structure information, in Å. Previously reported data are also tabulated, with their annotation numbers starting as T and E , for theoretical and experimental cases, respectively.

Metal	Structure a (c/a)	Surface	Relaxation			γ	τ	$\tau - \gamma$
			d_{12}	d_{23}	d_{34}			
La	hcp 3.77 (1.63)	(0001)	-4.77	4.33	-1.99	0.71 1.12 ^{T1} , 0.57 ^{T2} 1.02 ^{E1} , 0.85 ^{E2}	0.64	-0.07
Hf	hcp 3.19 (1.58)	(0001)	-6.86	3.49	-1.03	1.73 2.47 ^{T1} , 1.75 ^{T2} 1.79 ^{T3} , 2.15 ^{E1} 2.19 ^{E3}	1.24	-0.49
Ta	bcc 3.31	(100)	-13.43 -13.9 ^{T4} -6.3 ^{T5} -11±2 ^{E4}	0.09 0.15 ^{T4} -1.9 ^{T5} 1 ^{E4}	2.98 3.0 ^{T4} 1.9 ^{T5}	2.47 3.10 ^{T1} , 2.74 ^{T6} 2.27 ^{T4} , 3.59 ^{T7} 3.09 ^{T8}	1.78	-0.69
		(110)	-4.87 -5.1 ^{T4} -3.8 ^{T5}	0.24 0.06 ^{T4} 1.0 ^{T5}	0.01 -0.1 ^{T4} -0.5 ^{T5}	2.37 3.08 ^{T1} , 1.80 ^{T2} 2.31 ^{T4} , 2.58 ^{T6} 2.73 ^{T7} , 2.79 ^{T8} 3.15 ^{E1} , 2.90 ^{E3}	2.58	0.21
W	bcc 3.17	(100)	-12.16 -3.5 ^{T5} -4.02 ^{T9} -5.5 ^{T10} -6.33±6.33 ^{E5} -4.4±3.2 ^{E6} -11±2 ^{E7} -6 ~ ^{E8} -5.5±1.5 ^{E9} -6.7±2 ^{E10} -7.0±1.5 ^{E11} -6.0±1.5 ^{E12}	2.97 -0.6 ^{T5} 3.06 ^{T9} 2.4 ^{T10}	-1.34 1.2 ^{T10}	4.02 4.64 ^{T1} , 4.28 ^{T6} 3.86 ^{T7} , 4.05 ^{T8} 7.77 ^{T9} , 4.78 ^{T11} 6.0±0.9 ^{E13}	2.71 1.28 ^{T9} 1.28 ^{T12}	-1.31
		(110)	-3.76 -3.6 ^{T13} -4.1 ^{T14} -1.4 ^{T5} -0.8 ^{T9} -5.0 ^{T15} 0.0±3.0 ^{E14} -2.0 ~ ^{E15} 1.0±2.0 ^{E16} -3.1±0.6 ^{E17} -3.0±1.3 ^{E18} -2.2±1.0 ^{E19} -2.7±0.5 ^{E20}	0.45 0.2 ^{T13} -0.4 ^{T14} -0.4 ^{T5} 0.3 ^{T9} 4.6 ^{T15} 0.0±0.9 ^{E17} 0.2±1.3 ^{E18} 0.0±0.3 ^{E20}	0.02	3.28 4.01 ^{T1} , 3.84 ^{T2} 3.49 ^{T6} , 2.95 ^{T7} 3.47 ^{T8} , 5.08 ^{T9} 3.68 ^{E1} , 3.27 ^{E3}	4.08 2.72 ^{T9} 3.75 ^{T12}	0.80
Re	hcp 2.77 (1.62)	(0001)	-6.23 -6.03 ^{T16}	3.94 3.43 ^{T16}	-2.72 -1.75 ^{T16}	2.61 4.21 ^{T1} , 3.27 ^{T2}	3.37 3.54 ^{T16}	0.76

						2.94 ^{T3} , 3.77 ^{T17} 3.60 ^{E1} , 2.52 ^{E2} 3.63 ^{E3}			
Os	hcp 2.75 (1.58)	(10 $\bar{1}0$)	-16.44	0.12	-1.85				
		(0001)	-3.79	0.04	0.89	2.96	5.07	2.11	
						4.57 ^{T1} , 4.04 ^{T2} 3.45 ^{E1} , 3.44 ^{E3}			
Ir	fcc 3.88	(10 $\bar{1}0$)	-17.20	0.63	-2.41				
		(100)	-5.42	0.99	0.35	2.84	3.25	0.41	
			-2.7 ^{T5}	0.2 ^{T5}		3.72 ^{T1} , 3.81 ^{T2}	4.01 ^{T18}		
			-3.8 ^{T18}	1.0 ^{T18}	-0.5 ^{T18}	3.24 ^{T6} , 3.98 ^{T18}	6.36 ^{T22}		
			-6.56 ^{T19}			3.49 ^{T19} , 3.73 ^{T20}			
			-3.8 ^{T20}			3.74 ^{T22} , 2.90 ^{T23}			
			0.59 ^{T21}	0.0	-0.02	3.71 ^{T24}			
			-2±2 ^{E21}						
			(111)	-2.09	-0.51	0.32	2.06	4.37	2.31
				-1.5 ^{T5}	0.1 ^{T5}		2.97 ^{T1} , 3.41 ^{T2}	4.45 ^{T16}	
		-1.91 ^{T16}	-0.47 ^{T16}	0.22 ^{T16}	2.56 ^{T6} , 3.26 ^{T18}	4.87 ^{T18}			
		-1.3 ^{T18}	-0.2 ^{T18}	0.0 ^{T18}	3.00 ^{T20} , 3.26 ^{T22}	5.30 ^{T22}			
		-3.0 ^{T20}			2.82 ^{T23} , 3.02 ^{T24}	5.30 ^{T25}			
					3.27 ^{T25} , 3.00 ^{E1} 3.05 ^{E2} , 2.93 ^{E5}				
Pt	fcc 3.98	(100)	-2.54	-0.47	0.03	1.85	3.32	1.47	
			-4.1 ^{T5}	0.2 ^{T5}		2.73 ^{T1} , 2.48 ^{T2}	3.61 ^{T12}		
			-2.37 ^{T26}	-0.55 ^{T26}	0.29 ^{T26}	2.23 ^{T6} , 2.51 ^{T22}	5.59 ^{T22}		
			-2.11 ^{T27}	0.17 ^{T27}	-0.01 ^{T27}	2.65 ^{T24} , 1.81 ^{T26}	3.98 ^{T27}		
			0.2±2.6 ^{E22}			2.16 ^{T27} , 1.75 ^{T28}			
		(111)	0.99	-0.49	-0.12	1.49	4.25	2.76	
			-2.3 ^{T5}	0.2 ^{T5}		2.30 ^{T1} , 2.35 ^{T2}	5.24 ^{T12}		
			0.77 ^{T16b}	-0.23 ^{T16b}	-0.13 ^{T16b}	1.81 ^{T6} , 2.31 ^{T24}	4.45 ^{T16b}		
			0.85 ^{T26}	-0.56 ^{T26}	-0.15 ^{T26}	2.20 ^{T18} , 1.49 ^{T26}	5.61 ^{T25}		
			1.08 ^{T27}	-0.03 ^{T27}	0.00 ^{T27}	1.65 ^{T27} , 1.52 ^{T28}	6.67 ^{T27}		
			1.14 ^{T29a}	-0.29 ^{T29a}	-0.21 ^{T29a}	1.67 ^{T29a} , 2.23 ^{T29b}	5.60 ^{T34}		
			0.88 ^{T29b}	-0.22 ^{T29b}	-0.17 ^{T29b}	2.07 ^{T33} , 2.20 ^{T34}	6.28 ^{T35}		
			1.3 ^{T30}	0.3 ^{T30}	0.5 ^{T30}	2.48 ^{E1} , 2.49 ^{E2}	4.94 ^{T36}		
			1.20 ^{T31}	-0.50 ^{T31}		2.37 ^{E5} , 2.91 ^{E25}	2.57±0.40 ^{E26}		
	0.87 ^{T32}								
	1.1±0.44 ^{E23}								
	0.5±0.9 ^{E24}								
	1.4±0.9 ^{E25}								
Au	fcc 4.17	(100)	-1.52	0.10	0.32	0.86	2.07	1.21	
			-6.1 ^{T5}	0.5 ^{T5}		1.63 ^{T1} , 1.71 ^{T2}	3.14 ^{T22}		
			-1.0 ^{T20}			1.19 ^{T6} , 1.32 ^{T20}	2.06 ^{T27}		
			-1.51 ^{T26}	0.33 ^{T26}	0.24 ^{T26}	1.42 ^{T22} , 1.62 ^{T24}			
			-5.83 ^{T27}	1.19 ^{T27}	-0.23 ^{T27}	0.85 ^{T26} , 1.03 ^{T27}			
			-1.2 ^{T37}	0.4 ^{T37}		1.26 ^{T28} , 1.39 ^{T37}			
			-20±3 ^{E27}	2±3 ^{E27}					
		(111)	1.67	0.04	0.22	0.71	1.77	1.06	
			-3.7 ^{T5}	0.8 ^{T5}		1.28 ^{T1} , 1.61 ^{T2}	2.77 ^{T25}		
			-0.4 ^{T20}			1.01 ^{T6} , 1.32 ^{T20}	1.18±0.09 ^{E28}		

-0.04 ^{T26}	-1.86 ^{T26}	-1.40 ^{T26}	1.39 ^{T24} , 1.25 ^{T25}
-3.22 ^{T27}	0.58 ^{T27}	-0.10 ^{T27}	0.74 ^{T26} , 0.87 ^{T27}
0.8 ^{T38}	-0.3 ^{T38}		1.09 ^{T28} , 1.04 ^{T38}
			1.50 ^{E1} , 1.51 ^{E2}
			1.51 ^{E5}

- ^{T1} FCD-LMTO, GGA [4]
^{T2} TB LMTO, LDA [3]
^{T3} semi-empirical, EEM [60]
^{T4} PAW, GGA [188]
^{T5} TB [112]
^{T6} PAW, GGA (PBEsol) [49]
^{T7} semi-empirical, EEM [94]
^{T8} semi-empirical, second nearest-neighbor MEAM [95]
^{T9} modified LAPW, LDA [189]
^{T10} FP-LAPW, LDA [92]
^{T11} FP-LAPW, LDA [93]
^{T12} USPP, GGA (PBE) [115]
^{T13} FP-LAPW, LDA [190]
^{T14} FP-LAPW, LDA [191]
^{T15} TB [192]
^{T16} USPP, GGA (PW91) [109]
^{T16b} USPP, LDA [109]
^{T17} semi-empirical, MEAM [63]
^{T18} pseudopotential, LDA [193]
^{T19} pseudopotential, LDA [194]
^{T20} FP-LMTO, LDA [164]
^{T21} semi-empirical, MEAM [157]
^{T22} FP-LMTO, LDA [154]
^{T23} semi-empirical, MEAM [159]
^{T24} FKRR, LDA [64]
^{T25} pseudopotential, LDA [15, 195]
^{T26} USPP, GGA [20]
^{T27} semi-empirical, MEAM [11]
^{T28} semi-empirical, EESM [71]
^{T29a} FP-LAPW, GGA [19]
^{T29b} FP-LAPW, LDA [19]
^{T30} FP-LAPW, LDA [196]
^{T31} pseudopotential, GGA (PBE) [197]
^{T32} LCAO, LDA/GGA (PW91) [198]
^{T33} pseudopotential, LDA [199]
^{T34} LCAO, LDA [163]
^{T35} LCAO, LDA [200]
^{T36} pseudopotential, LDA [201]
^{T37} pseudopotential, LDA [202]
^{T38} pseudopotential, LDA [203]
^{E1} extrapolation from surface tension measurement [6]
^{E2} extrapolation from surface tension measurement [76]
^{E3} extrapolation from surface tension measurement [5]
^{E4} LEED [204]
^{E5} LEED [205]
^{E6} LEED [206]
^{E7} LEED [207]
^{E8} ion backscattering [208]
^{E9} LEED [209]
^{E10} LEED [210]
^{E11} spin-polarized LEED [211]
^{E12} LEED [212]
^{E13} spark discharge technique [213]
^{E14} LEED [214]
^{E15} HEIS [215]
^{E16} photoelectron diffraction [216]
^{E17} LEED [217]

- E18* LEED [218]
- E19* spin-polarized LEED [219]
- E20* surface XRD [220]
- E21* LEED [221]
- E22* HEIS [222]
- E23* LEED [223]
- E24* LEED [224]
- E25* MEIS [225]
- E26* lattice contraction experiment [148]
- E27* XRD [226]
- E28* lattice contraction experiment [227]

Table 5. Calculated surface relaxation (d_{ij}), surface energy (γ), and surface stress (τ) of light actinides. d_{ij} is given in percentage, γ and τ are in units of J/m². The calculated lattice constants a are listed with the structure information, in Å. Previously reported data are also tabulated, with their annotation numbers starting as T and E , for theoretical and experimental cases, respectively.

Metal	Structure a (c/a)	Surface	Relaxation			γ	τ	$\tau - \gamma$
			d_{12}	d_{23}	d_{34}			
Ac	fcc 5.66	(100)	-4.66	0.14	1.46	0.62	0.52	-0.10
		(111)	-4.28	1.94	0.17	0.73^{T1} 0.60, 0.87^{T1}, 0.82^{T2}	0.45	-0.15
Th	fcc 5.05	(100)	-2.74	1.72	-0.38	1.15	1.61	0.46
		(111)	-2.65	-0.71	-0.73	1.47^{T1} 1.05 1.48^{T1}, 1.37^{T2} 1.50^{E1}	0.90	-0.15
Pa	bct 3.93 (0.81)	(100)	-8.83	-1.70	2.23	1.70	1.49	-0.21
		(110)	-2.33	-0.01	0.94	2.58^{T1} 1.39 2.90^{T1}, 2.33^{T2*}	1.91	0.52

* calculated as fcc structure, for (111) plane

^{T1} FCD-LMTO, GGA [4]

^{T2} FCD-LMTO, LDA [48]

^{E1} extrapolation from surface tension measurement [5]

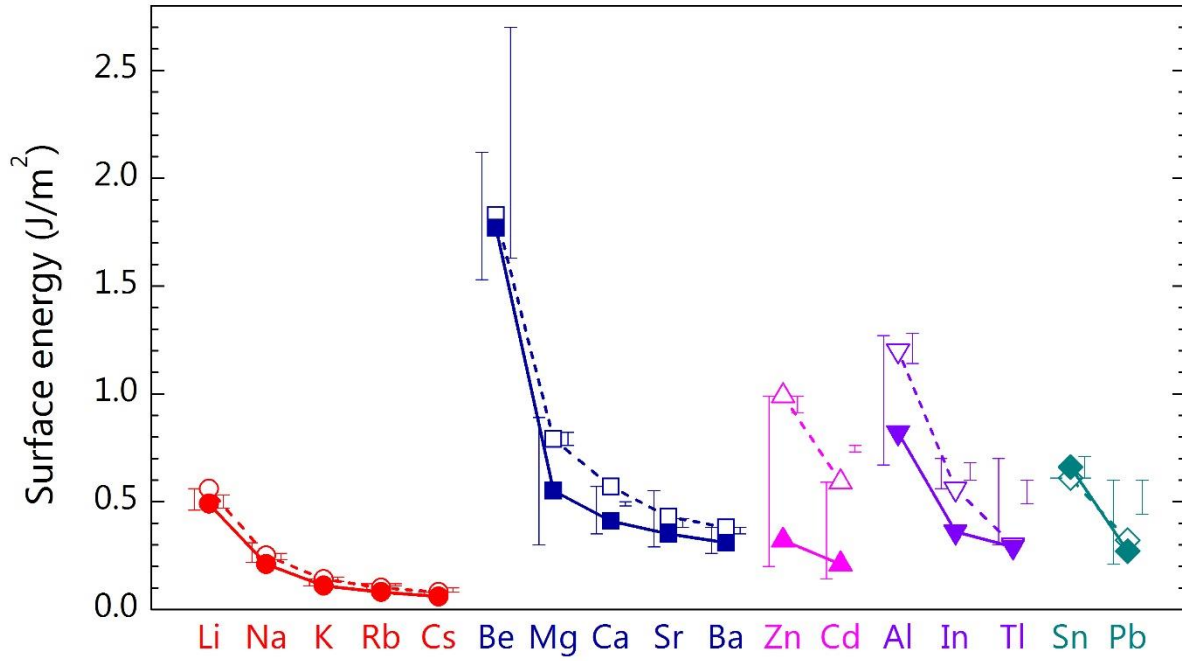


Figure 1. Theoretical surface energies of thermodynamically stable facets of low temperature crystallographic structures for simple metals. For comparison, the previous FCD-LMTO calculations [4] (dashed lines) are shown together, and the range of other theoretical and experimental data are also displayed on the left and right side of each surface energy plot, respectively. All previous data and the present calculation results demonstrate that the surface energy decreases as the atomic number increases, in each group of the periodic table.

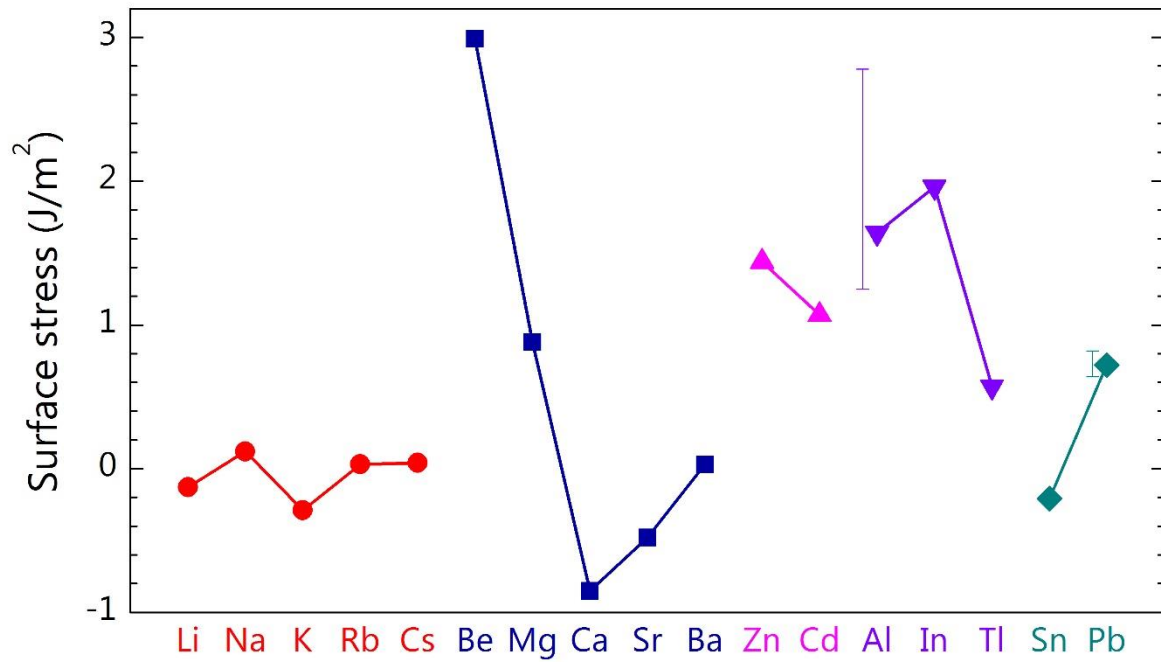


Figure 2. Theoretical surface stresses of thermodynamically stable facets of low temperature crystallographic structures for simple metals. For comparison, the range of previously reported theoretical data are shown together, if available. The trend of the present calculation results are somewhat scattered, but apparently have minimum values in the middle of the alkali and the alkali-earth group in the periodic table.

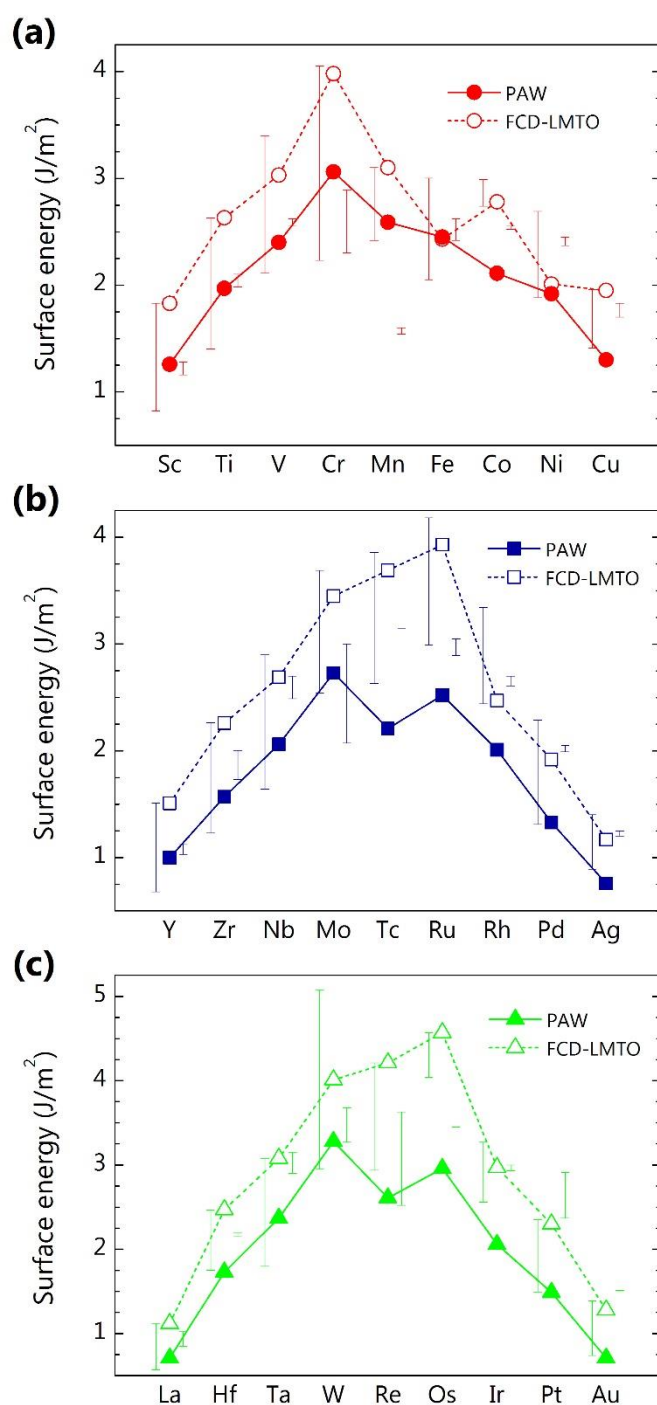


Figure 3. Theoretical surface energies of thermodynamically stable facets of low temperature crystallographic structures for the 3d (a), 4d (b), and 5d (c) transition metals, with surface energies from previous FCD-LMTO calculations shown for comparison. In addition, the ranges of the reported data from other theoretical and experimental approaches are marked on the left and right side of every surface energy plot, respectively. The surface energies vary approximately parabolically as a function of the d -electron occupation.

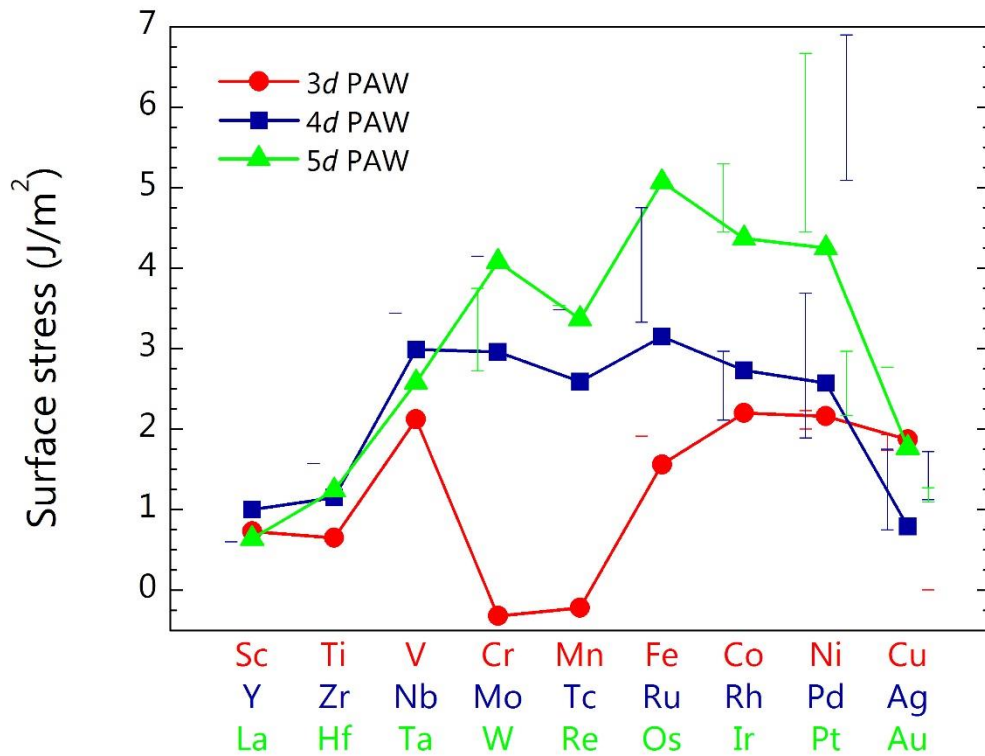


Figure 4. Theoretical surface stresses of thermodynamically stable facets of low temperature crystallographic structures for the transition metals. For comparison, the range of previously reported theoretical and experimental data are shown together, on the left and right side of each stress plot, respectively. The 4d and 5d curves are approximately parabolic-shaped with a shallow dip, while the curve of the 3d metals has a pronounced minimum. Moreover, Cr and Mn have negative values of the surface stress, which means that the (100) surfaces of Cr and Mn are under slight compression.